

# Whole Pattern Fitting and Rietveld Refinement

FILE: [fx 67 18A.raw] fx67 18A  
 SCAN: 4.0/70.0089/0.01995/71(sec), Co(35kV,40mA), I(p)=32390, 07/11/13 06:59p  
 PROC: [WPF Control File]

- |  |   |
|--|---|
| <input checked="" type="checkbox"/> K-alpha2 Peak Present      | [Diffractometer LP] Two-Theta Range of Fit = 4.0 - 70.0(deg)                                |
| <input checked="" type="checkbox"/> Allow Negative Isotropic B | <input checked="" type="checkbox"/> Specimen Displacement - Cos(Theta) = 0.066734(0.003199) |
| <input checked="" type="checkbox"/> Allow Negative Occupancy   | <input type="checkbox"/> Monochromator Correction for LP Factor = 1.0                       |
| <input checked="" type="checkbox"/> Apply Anomalous Scattering | <input type="checkbox"/> K-alpha2/K-alpha1 Intensity Ratio = 0.5                            |

Profile Shape Function (PSF) for All Phases: Pearson-VII, Fixed-BG, Lambda=1.78899Å (Co/K-alpha1)

Phase ID (7)	Source	I/Ic	Wt%	#L
Quartz - SiO <sub>2</sub>	PDF#04-008-7651	5.05(5%)	51.6 (3.1)	12
Orthoclase - KAlSi <sub>3</sub> O <sub>8</sub>	PDF#99-000-2749	0.90(5%)	20.9 (1.5)	8
Illite - KAl <sub>2</sub> (Si <sub>3</sub> Al)O <sub>10</sub> (OH) <sub>2</sub>	PDF#00-043-0685	0.50(5%)	12.0 (0.8)	46
Pyrite - FeS <sub>1.96</sub>	PDF#01-073-8127	2.66(5%)	6.4 (0.4)	8
Albite - NaAlSi <sub>3</sub> O <sub>8</sub>	PDF#04-007-5092	0.63(5%)	4.8 (0.4)	149
Natrolite - Na <sub>2</sub> (Si <sub>3</sub> Al <sub>2</sub> )O <sub>10</sub> ·2H <sub>2</sub> O	PDF#98-000-0325	0.90(0%)	3.8 (0.3)	188
Calcite - Ca(CO <sub>3</sub> )	PDF#04-007-4388	3.25(5%)	0.5 (0.2)	12

XRF(Wt%): Fe=3.0%, Ca=0.2%, K=4.1%, S=3.4%, Si=35.4%, Al=5.5%, Na=0.9%, O=47.4%, C=0.1%, H=0.1%

NOTE: Fitting Halted at Iteration 25(4): R=8.95% (E=2.54%, R/E=3.52, P=42, EPS=0.5)

